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Plasmonic nanopillar coupled two-dimensional random medium for broadband light trapping and harvesting

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Abstract. Random textures have proven to be a better option for light localization and energy harvesting in solar cells. On the other hand, plasmonic structures are significant in localizing the fields into submicron domains. We propose a layered structure design that contains the random dielectric medium with a plasmonic nanopillars array as a back reflector, followed by demonstrating its efficient light trapping ability through simulation means. This structure has shown significant enhancement in the broadband absorption of the light spectrum in the wavelength range UV-IR and a higher extinction in the near-infrared wavelengths. The structure also shows the dependence of reflection on the nanopillar height as well as localization in the nanopillar region. The broadened and red shifted plasmonic nanopillar resonances (transverse and longitudinal) in a high-index medium are shown as the reasons for enhanced broadband absorption. © 2015 Society of Photo-Optical Instrumentation Engineers (SPIE) [DOI: [10.1117/1.JNP.9.093061](https://doi.org/10.1117/1.JNP.9.093061)]

Keywords: random medium; nanopillars; broadband absorption; longitudinal plasmon resonance.

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1 Introduction

Nanophotonic structures have become one of the significant elements of light harvesting devices, such as thin-film solar cells, which are expected to offer better absorption enhancement and, hence, higher conversion efficiency.¹ The efficiency of the solar cell is dependent on absorption, surface volume recombination of the material, incident photon flux, and broadness of the light spectrum. Photonic structures in the solar cells are used to enhance the path length by trapping the light, whereas the surface and volume recombinations are controlled by the thickness. The short circuit current in the solar cell is determined by²

$$j_{sc} = e \int_0^{\infty} A(E) \frac{dN}{dE} dE = \int_0^{\infty} \frac{dj_{sc}}{dE} dE, \quad (1)$$

where j_{sc} , $A(E)$, dN/dE , and dj_{sc}/dE are the short circuit current, absorption, photon flux, and spectral broadness, respectively. The statistical ray trapping absorption limit or the Lambertian limit is given by³

$$A = 1 - \frac{1}{4L\alpha n^2}, \quad (2)$$

where $\alpha = 2\pi k/\lambda$ is the absorption coefficient, n and k are the real and imaginary parts of the refractive index of the material, and L is the material thickness. A structure that gives the absorption near to the Lambertian limit can enhance the solar cell efficiency. Hence, it is inferred that a photonic structure that can provide the necessary broadband (UV, visible, and IR) absorption through light localization with less recombination losses is desired for efficient solar energy

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harvesting. The research and development of thin-film solar cells has recently emerged again due to their low cost, lower volume recombination, and their potential to offer higher efficiencies.⁴ Theoretical and experimental investigations have been carried out on various photonic structures, such as periodic,⁵ random,⁶ quasirandom,⁷ and plasmonic structures,^{8–10} for solar cell applications. Still, the quest continues for a solar cell configuration of improved efficiency.

In particular, the medium with a randomly varying refractive index introduces multiple scattering conditions to the incident light, which eventually leads to many interesting phenomena, such as enhanced absorption, light localization, hyper transport (stochastic acceleration), random lasing, etc.¹¹ As far as the solar energy harvesting is concerned, random structures are noted for broadband light absorption and antireflection. Gaussian random structures are especially reported to enhance the performance of the device.¹² In addition to solar energy harvesting, localization of light in random media finds applications in imaging, nano lasing (sensors), and quantum information processing.^{13,14} The main challenge from the application point of view is to localize the light in a thin medium, which is not possible with a dielectric random medium alone. The solution lies in the use of plasmonic nanostructures with high near-field spectral densities, inside the thin dielectric random medium.

Plasmonic structures with large evanescent electromagnetic (EM) fields can squeeze the incident light fields into subwavelength domains. Hence, the plasmonic structures became a competent peripheral in a solar cell, such as top surface, solar concentrator,¹⁵ and back reflector.^{16–19} The extended plasmonic structures, especially nanorods, wires, and pillars with dual mode (transverse and longitudinal) plasmon resonances, are the structures of importance in light harvesting.²⁰ The localized surface plasmon resonance (LSPR) and SPR properties are modulated by tuning the size, aspect ratio, and separation of these extended plasmonic structures. The longitudinal resonance mode depends on the precise length of the structure.²¹ The plasmonic near-field strength varies as a function of size in the nano regime²² and plasmon resonance shift and broadening take place depending on the separation.²³ In addition, plasmon resonance is sensitive to the refractive index of the surrounding medium or interface material. Based on these advantages, the extended plasmonic structural arrays are reported to be efficient for surface enhanced raman scattering²⁴ substrates, some frequency generation enhancement,²⁵ biosensing,²⁶ light trapping, and broadband absorption.²⁷ Hence, the combined effect of random and periodic media on the EM wave (mentioned in the paper) and using the extended plasmonic structures (nanopillars) at the back reflector to exploit the dual plasmon resonances (longitudinal and transverse) for light trapping. Degeneration or separation of transverse and longitudinal plasmon modes due to the Si surrounding medium establishes a new way to broaden the spectral response of the structures.

In this paper, we propose the design of an Si random medium with a plasmonic nanopillar array as a back reflector and demonstrate the strong broadband localization (high absorption) properties by finite-difference time domain (FDTD) numerical simulation. First, the contribution of the random medium to reduced reflection and reflection properties of the Si random medium with different back reflectors is presented. Further, based on the reflection properties, a random structure with a nanopillar back reflector is analyzed in terms of light propagation, plasmon coupling, and overall absorption. The properties of this structure are also analyzed with respect to pillar height. The structure under consideration is shown to exhibit broadband localization properties with high absorption and is expected to be good for high-efficiency solar cell fabrication.

2 Effect of Two-Dimensional Random Medium on Optical Properties of a Thin Si Film

The proposed design of the random structure with a back reflector is shown in Fig. 1(a), where the thickness, length, and width of the simulated structure are 0.6, 1.5, and 1.5 μm , respectively. Here, random media can be characterized only by the random medium parameters in the simulation, such as the refractive index (3.46) of Si, thickness of the random medium 0.25 μm , average amplitude of the spike in the random medium 0.1 μm , the sampling resolution of the surface ~ 30 nm, and the average correlation length X, Y axis-10 nm. Silver (Ag) is considered as a material for the back reflector. The simulations are performed using FDTD (*Lumerical*). The simulation parameters considered in the study are as follows: dimension is three-dimensional,

Fig. 1 (a) The proposed design of silicon random medium with a planar back reflector, (b) plot: reflection as a function of wavelength of flat (black curve) and random (red curve) surface Si block, and (c) plot: absorption as a function of wavelength in Si with flat (black curve) and random (red curve) surfaces.

background index is 1, simulation time is 500 fs, simulation region size is $x = 1.3 \mu\text{m}$, $y = 1.3 \mu\text{m}$, $z = 0.8 \mu\text{m}$, and the minimum mesh cell size (grid size) is 1 nm. The boundary conditions used here are perfectly matched layer with a layer number of 12. These are also incorporated in the manuscript. The broadband source (0.2 to $1.5 \mu\text{m}$) is applied on to the structure [Fig. 1(a)] through a two-dimensional (2-D) field monitor (for reflection and incident field measurement) and the transmitted field is measured by another 2-D field monitor placed just before the back reflector. The light transport scenario inside the structure is observed by placing 2-D cross-sectional field monitors at subsequent propagation distances of 0.1, 0.2, 0.3, 0.4, and $0.5 \mu\text{m}$, respectively, from the plane of incidence. The random 2-D surface texture with specific features is chosen using the inbuilt structures from the software.

Figures 1(b) and 1(c) show that the reflection in the UV and visible regions is greatly reduced after introducing randomness on the surface of Si, hence, the absorption is improved. The plane wave incident on the random surface cannot propagate ballistically and undergoes multiple scattering in random directions, which reduces the reflection. The randomized light penetrates through the Si and is incident on the back reflector at different angles, which increases the path length of the light through the structure and improves the absorption. Figures 1(b) and 1(c) also clarify that the IR region is least affected by the random medium. According to the Mie scattering theory, the scattering wavelength depends on the size and refractive index of the scatterer, which is the reason why the 2-D random medium does not have much effect on the IR region. Further, to reduce the reflection in the IR region and improve the broadband absorption, the plasmon approach is adopted by replacing the planar back reflector with a structured back reflector.

3 Random Si Structure with Different Back Reflectors

The reflections from the Si random medium with different back reflectors are measured by the same simulation approach. The shape and geometry of the Ag back reflectors used in this study

Fig. 2 The reflection spectra from Si random structure with (a) planar, (b) saw tooth, (c) sinusoidal, and (d) nanopillar back reflectors.

are planar (S1), saw tooth (S2), sinusoidal wavy (S3), and nanopillar (S4) with a thickness of 50 nm and a 40 nm feature (pillar, saw tooth, or sin wavy) on 10 nm plane Ag. The reflection spectra of the Si random medium with different back reflectors (S1, S2, S3, and S4) are shown in Figs. 2(a)–2(d), respectively. The integrated area under the reflection spectrum of each structure (S1, S2, S3, and S4) indicates the magnitude of the broadband reflection. Among all of these, the structure with the nanopillar back reflector (S4) has resulted in the lowest broadband reflection as shown in Fig. 2(d). Specifically, a well-suppressed IR reflection is observed in structure S4 compared to the others, which is advantageous for IR light harvesting.

A thorough inspection of Fig. 2 illustrates the idea that there is a systematic reduction in reflection from planar (S1) → sinusoidal (S3) → saw tooth (S2) → nanopillar (S4) back reflector structures. The structures with sharp edges, such as S2 and S4, exhibit better reduced reflection properties, which could be due to the formation of the plasmonic hotspots (high spectral density regions) at sharp metal edges. Moreover, nanorods or nanopillar structures are unique due to their double plasmon resonances (transverse and longitudinal). Hence, the Si random medium with a nanopillar back reflector is considered for further studies.

4 Si Random Structure with Nanopillar Back Reflector for High Absorption and Light Localization

An Si random structure with an Ag back reflector with an increased nanopillar height (from 40 to 200 nm) is shown in Fig. 3(a). The lattice parameters of the nanopillar array are 40 nm, 40 nm in the x and y directions, respectively. The reflection from the structure is further reduced upon increasing the nanopillar height [Fig. 3(b)], almost in every region (UV-VIS-IR). This structural feature avoids the necessity of separate antireflection coatings if implemented in the solar cell fabrication. Figure 3(c) shows the vertical cross-sectional view of the field enhancement in this structure, from which it is clear that the fields are mostly accumulated with significant enhancement in the random medium, nanopillar surfaces, and middle region of the nanopillar array. As

Fig. 3 (a) The random structure with nanopillar back reflector, (b) the reflection spectra of the structures with 40 nm (red curve) and 200 nm (black curve) nanopillar height, (c) the vertical cross-sectional field profile, (d) the absorption spectrum of the structure, the field distributions at (e) 0.1 μm , (f) 0.2 μm , (g) 0.3 μm , (h) 0.4 μm , and (i) 0.5 μm propagation distances from incident plane.

expected from Fig. 3(d), the absorption by the structure is significantly improved over the broad wavelength range of the visible to IR regions. Figure 3(d) also shows a comparison among flat Si, Si random medium, flat Si with nanopillar back reflector. Among all of these, the random Si with the nanopillar back reflector is dominant in absorption. The Fabry-Perot oscillations due to the thinness of the Si substrate are effectively suppressed by the random medium. Another important point to be noted from Fig. 3(d) is that the UV-visible absorption enhancements are collectively driven by random and plasmonic media, whereas absorption enhancements in the IR region are driven very strongly by the plasmonic medium.

To understand the origin of absorption enhancement, the light transport scenario inside the structure is studied. The propagation of the broadband light through the structure is observed at certain propagation distances, 0.1, 0.2, 0.3, 0.4, 0.5, and 0.6 μm , from the plane of incidence. Figures 3(e)–3(i) are the field distributions (horizontal cross-section) at the propagation distances of 0.1, 0.2, 0.3, 0.4, and 0.5 μm , respectively. At the distance of 0.1 μm , the field is randomized by the Si random medium and accumulates at certain spots. Due to multiple scattering in the random medium, the field is prompted to travel in channels that are observed at a 0.2 μm distance. The randomized light enters and is incident on the plasmonic nanopillar surfaces at different angles, which excites the localized surface plasmons (transverse modes) on the nanopillar surfaces. Simultaneously, the light entering into the nanopillar region is strongly affected by longitudinal surface plasmons (surface plasmon polariton) along the length of the nanopillar, which is evident from Figs. 3(h) and 3(i). It is interesting that the field enhancements are

Fig. 4 The absorption curves at different propagation distances of (a) 0.1 μm (black), 0.2 μm (red), 0.3 μm (blue), 0.4 μm (green), and 0.5 μm (magenta), 0.6 μm (pale green) and the Lambertian absorption limit (navy blue). (b) The normalized absorption as a function of wavelength at different nanopillar heights (20, 30, 80, 120, and 160 nm). (c) The plot showing the extinction of the nanopillar array (200 nm) with different background index media (refractive index 1, 1.5, 2, 3.46).

maximum at 0.4 μm [Fig. 3(h)] and 0.5 μm [Fig. 3(i)] distances and the accumulated field (mostly at the middle area) at 0.4 μm is dispersed across more area at 0.5 μm . This analysis is further supported by the absorption calculated [shown in Fig. 4(a)] at the respective propagation distances of 0.1, 0.2, 0.3, 0.4, 0.5, and 0.6 μm (front face of the metal back reflector plate). Figure 4(a) indicates that the absorption increases with the propagation distance. Due to the randomization, there is $\sim 10\%$ absorption, whereas after entering the periodic nanopillar zone, there is a drastic variation in absorption (up to 80%); these are compared with the Lambertian curve (navy blue).

Analysis of Figs. 3(c), 3(h), and 3(i) clearly indicates the light localization conditions prevailing in the nanopillar region, which is also supported by a drastic increment in absorption [Fig. 4(a)] between 0.4 and 0.5 μm propagation distances. From Fig. 4(a), it is clear that at the 0.3 to 0.4 μm distance, there is a significant improvement in absorption, which could be due to the localized plasmons on the nanopillar surface. Second, there is a large absorption enhancement within the next 100 nm (from 0.4 to 0.5 μm), which is due to longitudinal plasmonic modes (surface plasmon polariton). Based on the fact that the longitudinal resonances depend on the length of the nanopillar, absorption properties of the present structure at nanopillar heights of 200 nm (4040200), 120 nm (4040120), 80 nm (4040080), 30 nm (4040030), and 20 nm (4040020) are calculated and plotted in Fig. 4(b). It is clear from Fig. 4(b) that only at the 20 nm pillar height are the plasmon effects completely suppressed, which indicates the absence of longitudinal surface plasmons. The presence of longitudinal surface plasmons is indicated by a drastic increase in absorption by the structure when the nanopillar height is increased from 20 to 30 nm [Fig. 4(b)].

However, the origin of the improved IR and broadband absorptions in this structure are still unclear. To understand this, one has to consider the surrounding environment of the plasmonic

nanopillar array. In the present structure, the nanopillar region is intruded into silicon, which means that there is a certain effect of the surrounding medium (Si) on the plasmonic properties. The analysis of the background index effect on the plasmon resonances has revealed a very interesting point of plasmonic resonance broadening and red shifting as shown in Fig. 4(c). The normalized plasmon resonances for different background refractive indices are plotted, where the plasmon resonance of the nanopillar array is broadened and red shifted with an increase in the surrounding medium refractive index. When the refractive index of the surrounding medium is 1 (free space), the resonance occurs at ~ 400 nm (black curve), whereas when the surrounding medium refractive index is increased to 1.5 and 2, the curve broadens and is red shifted. In addition, there are multiple peaks occurring (red and blue curves) at 1.5 and 2 refractive indices, which are the transverse and longitudinal modes as expected. When Si is taken as the surrounding medium for the Ag nanopillar array, the plasmon resonance broadens and the plasmonic wavelengths are red shifted such that the transverse mode is in the visible region and the longitudinal mode is in the IR region. Hence, the broad and red shifted plasmonic nanopillar resonances (transverse and longitudinal) in the Si medium are the origin of higher enhancements in IR and broadband absorption.

5 Conclusion

In conclusion, ultrathin ($0.6 \mu\text{m}$) Si random structures with different back reflectors are analyzed through FDTD simulation. Among all the different structures considered in the analysis, the nanopillar structure was found to offer the lowest reflection with high broadband absorption. In the same structure, the dependence of reflection on nanopillar height is demonstrated. Further, plasmon affected localization in the proposed structures with chosen features is observed. Hence, the analysis reveals that the structure is advantageous due to its random textured surface, which increases the UV-Visible path lengths and the absorption. Further, it is inferred that the plasmonic nanopillars in the high-index surrounding medium (Si) are efficiently trapping the broadband randomized light through their red shifted and broadened plasmon resonances (transverse and longitudinal). Hence, the structure with random and plasmonic features, if integrated, is expected to offer significant broadband (localization) absorption and, in turn, improved conversion efficiency in thin-film solar cell structures.

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